

General Disclaimer

One or more of the Following Statements may affect this Document

- This document has been reproduced from the best copy furnished by the organizational source. It is being released in the interest of making available as much information as possible.
- This document may contain data, which exceeds the sheet parameters. It was furnished in this condition by the organizational source and is the best copy available.
- This document may contain tone-on-tone or color graphs, charts and/or pictures, which have been reproduced in black and white.
- This document is paginated as submitted by the original source.
- Portions of this document are not fully legible due to the historical nature of some of the material. However, it is the best reproduction available from the original submission.

THE CALCULATION OF
THEORETICAL CHROMOSPHERIC MODELS AND
PREDICTED OSO I SPECTRA

NASA Grant NSG-7054

Progress Report No. 1

For the period 1 July 1974 to 31 December 1975

Principal Investigator

Eugene H. Avrett

March 1976

Prepared for

National Aeronautics and Space Administration
Washington, D.C. 20546

Smithsonian Institution
Astrophysical Observatory
Cambridge, Massachusetts 02138

The Smithsonian Astrophysical Observatory
and the Harvard College Observatory
are members of the
Center for Astrophysics

The NASA Technical Officer for this grant is Dr. Adrienne F. Timothy, Code SG,
Headquarters National Aeronautics and Space Administration, Washington, D.C. 20546

N76-21110

Unclas
21459

G3/92

(NASA-CR-146772) THE CALCULATION OF
THEORETICAL CHROMOSPHERIC MODELS AND
PREDICTED OSO I SPECTRA Progress Report, 1
Jul. 1974 - 31 Dec. 1975 (Smithsonian
Astrophysical Observatory) 24 p HC \$3.50



THE CALCULATION OF
THEORETICAL CHROMOSPHERIC MODELS AND
PREDICTED OSO I SPECTRA

NASA Grant NSG-7054

Progress Report No. 1

For the period 1 July 1974 to 31 December 1975

Principal Investigator

Eugene H. Avrett

March 1976

Prepared for .

National Aeronautics and Space Administration
Washington, D.C. 20546

Smithsonian Institution
Astrophysical Observatory
Cambridge, Massachusetts 02138

The Smithsonian Astrophysical Observatory
and the Harvard College Observatory
are members of the
Center for Astrophysics

The NASA Technical Officer for this grant is Dr. Adrienne F. Timothy, Code SG,
Headquarters National Aeronautics and Space Administration, Washington, D.C. 20546

TABLE OF CONTENTS

	<u>Page</u>
ABSTRACT.....	v
1 INTRODUCTION.....	1
2 SOLAR MODEL.....	3
3 SPECTRUM SYNTHESIS PROGRAM.....	5
4 COMPUTING AT NCAR.....	10
5 SPECTRUM CALCULATION.....	11
6 FURTHER WORK.....	19
7 REFERENCES.....	20

ABSTRACT

We report our progress in computing theoretical solar chromospheric and photospheric models for use in analyzing OSO 8 spectra. We have updated the Vernazza, Avrett, and Loeser (1976) solar model and produced self-consistent non-LTE number densities for H I, He I, He II, C I, Mg I, Al I, Si I, and H⁺. These number densities have been used in the calculation of a theoretical solar spectrum from 90 to 250 nm, including approximately 7000 lines in non-LTE. More than 60,000 lines of other elements were treated with approximate source functions.

PRECEDING PAGE BLANK NOT FILMED

THE CALCULATION OF THEORETICAL CHROMOSPHERIC MODELS AND PREDICTED OSO I SPECTRA

NASA Grant NSG-7054

Progress Report No. 1

1. INTRODUCTION

The OSO 8 experiment has observed radiation from different regions on the solar disk and, through spectrum scans, has probed a range of depths in the atmosphere from the corona to the upper photosphere. These observations, together with earlier Skylab and rocket observations, should lead to a new and greatly improved understanding of the structure and behavior of the solar atmosphere and of the heating of the corona, as well as to significant advances in our theoretical understanding of high-temperature plasmas.

The variation with depth of temperature, density, and other atmospheric parameters at a given point on the disk can be determined from the emergent spectrum. However, the computations necessary to derive these parameters require a major effort. We have developed a two-stage procedure for computing theoretical solar chromospheric and photospheric spectra. In the first, we construct a solar model based on the non-LTE computer program PANDORA (see Avrett and Loeser, 1969; Avrett, 1971; Vernazza, Avrett, and Loeser, 1973).

In the second stage of the spectrum calculation, we make use of a spectrum-synthesis program written by Kurucz (1974) and based upon his model atmosphere program ATLAS (1970), which includes data for 300,000 lines computed by Kurucz and Peytremann (1975). The statistical-equilibrium number densities from the model calculation are used to determine the non-LTE line source functions of the abundant elements, while the less abundant ones are treated with approximate source functions.

In the next section we describe our current solar model; and in section 3 we outline various developments in the spectrum synthesis program, especially the treatment of lines merging into continua and non-LTE modifications to the basic programs. In sections 4 and 5 our spectrum calculations are described. Finally, we discuss further work to remedy shortcomings in the most recent calculations.

2. SOLAR MODEL

We construct a solar model by choosing a temperature-height distribution such that the computed emergent intensity is in best agreement with observed line and continuum spectra in the ultraviolet, visible, and infrared spectral regions. PANDORA is used to solve the radiative-transfer and statistical-equilibrium equations for hydrogen, helium, carbon, silicon, and other important constituents. The model calculation is iterative in that only one atom can be computed at a time, while others are held fixed. Thus a self-consistent solution is found by cycling through the atoms several times, updating the number densities with each calculation.

Vernazza, Avrett, and Loeser (1976) have completed a detailed study of the solar continuous spectrum redward of 125 nm. They have constructed a temperature-density model, which is a representation of the quiet solar atmosphere in the height range between the photosphere and the chromosphere-corona transition region. We have revised and improved that model to obtain the temperature-height relation shown in Figure 1. The model is self-consistent in H I, He I, He II, C I, Mg I, Al I, Si I, and H⁻.

We expect to further revise this model by studying the differences between our calculated spectrum and the rocket and OSO observations all through the ultraviolet and the Skylab spectra below 140 nm.

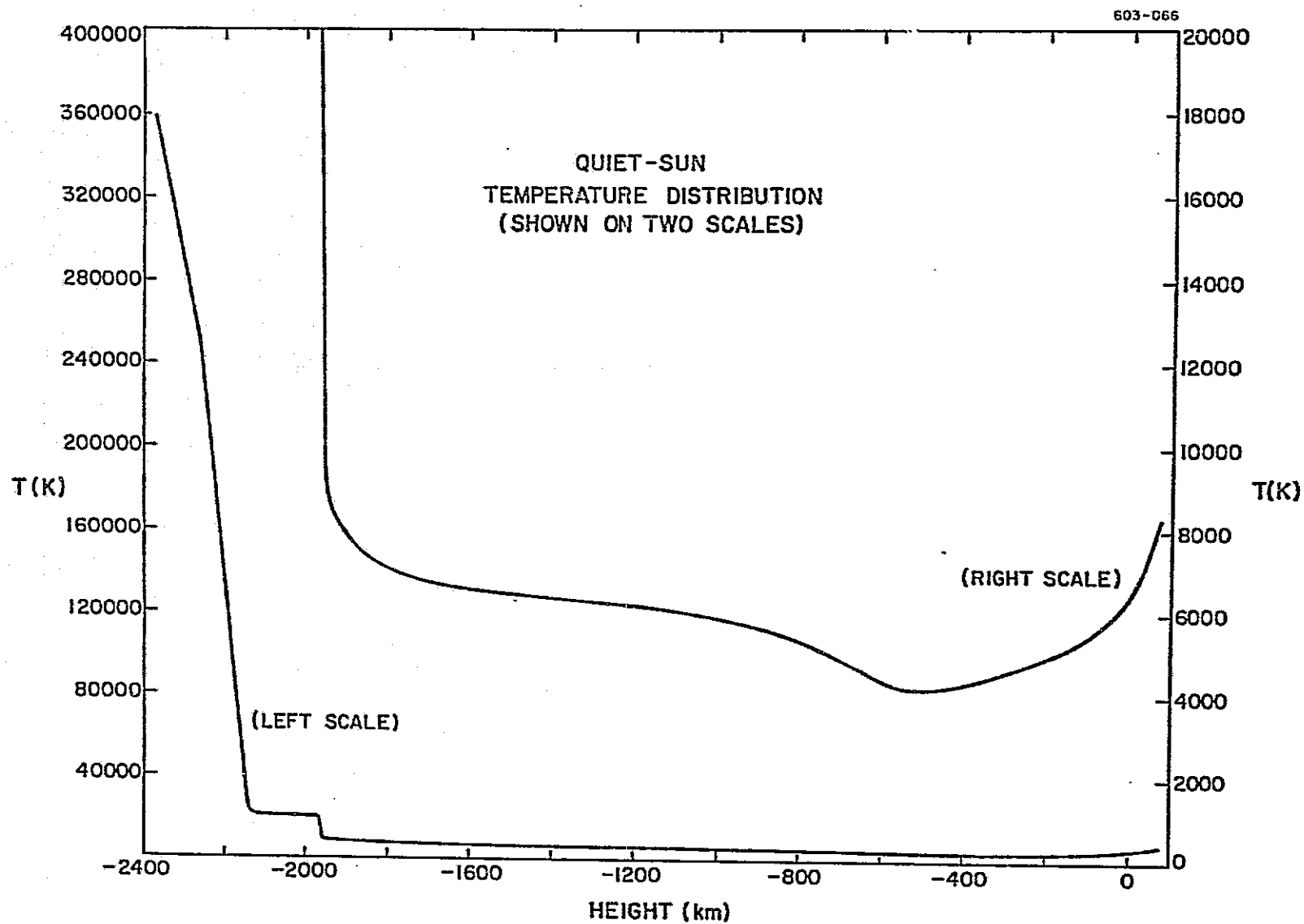


Figure 1. The temperature-height relation for our revised solar model.

3. SPECTRUM SYNTHESIS PROGRAM

We have continually improved our spectrum synthesis programs during the course of this research. The basic spectrum synthesis program works as follows. For a given model atmosphere tabulated at 40 depths, we compute number densities and partition functions for all atoms and ions. Then we read the magnetic tape that lists the gf values calculated by Kurucz and Peytremann (1975), and compute a line opacity spectrum at each depth. The expressions for radiative, Stark, and van der Waals broadening are

$$\Gamma_R = \Gamma_{\text{classical}} = 2.223E13/\lambda^2, \quad \lambda \text{ wavelength in nm} ;$$

$$\Gamma_S = 1.0E-8 n_{\text{eff}}^5 N_e ;$$

$$\Gamma_W = 4.5E-9 \langle r^2 \rangle^{4/10} [N_H + 0.42 N_{He} + 0.85 N_{H_2}] (T/10000)^{3/10} ;$$

where

$$\langle r^2 \rangle = 2.5 n_{\text{eff}}^2 / Z_{\text{eff}}^2 ,$$

$$n_{\text{eff}}^2 = R Z_{\text{eff}}^2 / E_{\text{up}} ,$$

Z_{eff} is the charge plus 1, E_{up} is the upper level energy, and R is the Rydberg energy. Next the continuum opacities, source functions, and intensities are evaluated at several points in the wavelength interval. The continuum quantities are interpolated to each point in the spectrum; the line opacity is added; the source function is approximated by

$$[(\kappa + \sigma)S_{\text{cont}} + \ell S_{\text{line}}]/(\kappa + \sigma + \ell) ;$$

and the emergent spectrum is computed. Here κ and σ are the continuous absorption and scattering coefficients, ℓ is the line absorption coefficient, S_{cont} is the continuum source function including scattering, and S_{line} is the line source function, which is assumed to be the Planck function.

The following improvements have been made. We have computed mean square radii for the 4p orbitals of the iron group atoms and ions, and produced an interpolation formula

$$\langle r^2 \rangle = (45 - A + Z)/(Z + 1)$$

where A is the atomic number and Z is the charge. This expression is used for van der Waals broadening of all iron group atoms, assuming that the strong lines are all resonance lines with a 4p upper state.

There is now provision for additions, deletions, and corrections to the table of gf values and for use of individual "real" radiative, Stark, and van der Waals damping constants for each line.

To resolve the contribution of individual lines to blends, we now compute, in addition to the spectrum, the central intensity for each line in isolation.

We automatically produce spectrum plots with identifications.

The two most important advances as far as improving the appearance of the calculated spectrum have been treatment of lines merging into continua and the development of a procedure for computing thousands of lines in non-LTE.

One of the obvious faults in the preliminary calculations made one year ago was that strong discontinuities appeared at the C I, Si I, Al I, and Mg I edges, whereas the real spectrum makes smooth transitions from one continuum to another because in the real spectrum there are numerous lines that gradually merge into each continuum. In rewriting the opacity routines to include departures from LTE as discussed below, photoionization continua were put in for level-to-level transitions rather than

for term-to-term transitions as was the case previously. Thus, for example, for C I and Si I, ionization from the neutral ground term 3P to the ionized ground term 2P actually forms 6 continua, $^3P_0 \rightarrow ^2P_{1/2}$, $^3P_0 \rightarrow ^2P_{3/2}$, $^3P_1 \rightarrow ^2P_{1/2}$, $^3P_1 \rightarrow ^2P_{3/2}$, $^3P_2 \rightarrow ^2P_{1/2}$, $^3P_2 \rightarrow ^2P_{3/2}$. Each of these continua has a series of lines converging up to it. The lines merge into a quasi-continuum at an upper energy or upper quantum number determined by Stark broadening, because lines are no longer visible when the Stark width exceeds the line spacing. In practice, at each depth in the atmosphere, we compute the energy at which individual lines are no longer visible and extend each continuum redward at a constant level to this point. This technique smooths the transition from one continuum to another even if no lines are included explicitly.

For Al I and Mg I we were able to compute Rydberg series to high n (80), and to find or estimate the radiative, Stark, and van der Waals broadening for each line. For Si I and C I there is so much configuration interaction that extrapolated energy levels can be off by up to 2 cm^{-1} unless great effort is made to include the interaction effects, so we were not able to compute the series. For Si I, however, energy levels have been observed up to $n = 56$ although many of them were unclassified. We were able to pick out the interacting levels by estimating the mutual repulsion, so we could assign each level to an LS series. Then we estimated LS f values by extrapolating each series. These f values will be correct for many of the lines but wrong for the strongly interacting lines. However, the total f values spread over all transitions should be correct as configuration interaction only redistributes the line strengths.

To demonstrate the improvement in the new calculations we show in Figure 2 sample old and new spectra calculated around the Si I edge at 198 nm. The old calculation predicted an abrupt discontinuity, and the new one, a gradual slope, in agreement with the observations.

To treat the non-LTE effects we have rewritten ATLAS (Kurucz, 1970) routines for partition functions and for continuous opacity from H I, He I, He II, C I, Mg I, Al I, and Si I to produce non-LTE populations, opacities, and source functions. We have added a new line opacity routine that produces non-LTE opacity and a source function for each C I, Mg I, Al I, and Si I line. The changes were accomplished by inserting departure coefficient b 's as follows.

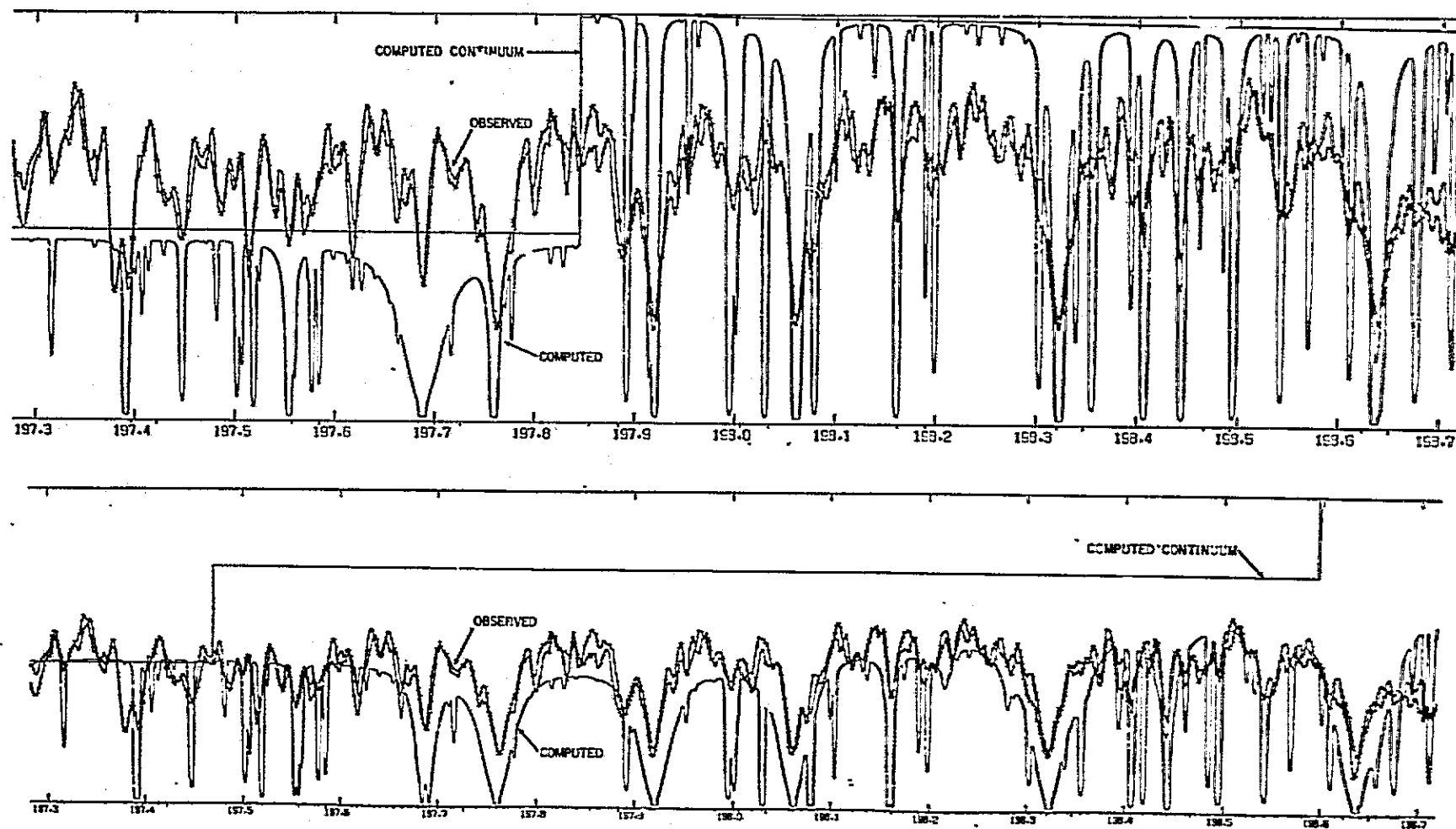


Figure 2. (a) A previous calculation showing the silicon discontinuity at 197.8 nm. Also shown are two Harvard rocket scans by Kohl, Parkinson, and Reeves that do not show an abrupt discontinuity. The vertical scale is linear but in arbitrary units. (b) Our most recent calculation showing the smooth transition across this region, in agreement with the observations, which results from treatment of lines merging into the continuum.

Partition functions:

$$U = \sum g_i e^{-E_i/kT} \rightarrow \sum g_i b_i e^{-E_i/kT}$$

where g_i and E_i are the statistical weight and energy for each level;
Boltzman factors:

$$\frac{N_i}{N} = \frac{g_i}{U} e^{-E_i/kT} \rightarrow \frac{b_i g_i}{U} e^{-E_i/kT}$$

where N and N_i are the total and level number densities;
Stimulated emission:

$$1 - e^{-h\nu/kT} \rightarrow 1 - \frac{b_{up}}{b_{lo}} e^{-h\nu/kT}$$

where up and lo refer to the upper and lower levels. For ionization, up refers to the ground state of the ion.

Source functions:

$$S(lo \rightarrow up) = \frac{2h\nu^3}{c^2} \left[e^{h\nu/kT} - 1 \right]^{-1} \rightarrow \frac{2h\nu^3}{c^2} \left[\frac{b_{lo}}{b_{up}} e^{h\nu/kT} - 1 \right]^{-1} .$$

In practice, b 's are calculated only for the lowest 6 to 10 terms, so for higher levels b 's are assumed to have the same value as the b for the lowest level of the ion.

4. COMPUTING TIME AT NCAR

This work on spectrum synthesis has been exceedingly difficult, requiring innovations and much more sophisticated programing than originally envisioned. Furthermore, calculation of the spectrum in non-LTE requires a great deal of computer time, even for debugging. Because of limited funds provided by the grant for computing, we have to use free computing where available. Fortunately we have been able to use the CDC 7600 at the National Center for Atmospheric Research through collaboration with Oran R. White of the High Altitude Observatory. A considerable inconvenience of working at NCAR is that to check the calculations we must bring magnetic tapes back to Cambridge to plot the spectra because NCAR does not have plotting facilities.

5. SPECTRUM CALCULATION

We used the model described in section 2 and the program described in section 3 to compute the theoretical solar spectrum from 90 to 250 nm including non-LTE effects for H I, He I, C I, Mg I, Al I, Si I, and H⁺. We computed approximately 7000 lines in non-LTE. More than 60000 lines of other elements were treated with approximate source functions.

In Figure 3 we show an enlargement of Figure 2b with line identifications. Of the many lines included in the calculation, only those with residual intensities less than 0.99 are indicated. There are numerous non-LTE Si I lines in this region. The lines that show up prominently with triangular shapes in both the observed and calculated spectra are Si I resonance lines.

In Figure 4 we show a small region of chromospheric spectrum at 149.3 nm where the lines appear in emission.

Figure 3. The calculated spectrum compared to the Harvard rocket spectra of Kohl, Parkinson, and Reeves for the region 197.6 to 199.1 nm. The observed and computed spectra are not plotted on the same vertical scale; the two scales are linear but arbitrary. This figure shows approximately the same wavelength region as Figure 2b but enlarged to show detail and with line identifications added. The identifications at the top of the figure include: the last three digits of the wavelength, the element identification and charge (atomic number before decimal point, charge after; thus 14.00 = Si I and 28.01 = Ni II), then, the lower energy level in cm^{-1} , and finally the fraction of the full scale in per mil for the center of each line if it were in isolation. Thus strong lines have small central intensities and weak lines have values near the continuum, which is indicated. The numerous Si I lines are computed in non-LTE.

161 27.01 15394 583	12 14.00 15394 537
207 14.00 15394 261	
285 25.01 21581 551	203 14.00 15394 505
404 27.00 15394 742	
420 14.00 15394 517	412 14.00 15394 235
647 14.00 15394 505	528 14.00 15394 218
805 14.00 15394 599	800 14.00 15394 159
918 25.01 19041 517	917 27.01 10748 734
973 23.01 19112 554	971 25.01 31661 511
1185 14.00 15394 551	150 25.01 21711 118
	175 14.00 15394 185
	205 14.00 15394 77 9
249 14.00 15394 522	453 14.00 15394 150
323 25.01 27820 439	
	514 25.01 35252 720
602 14.00 15394 151	815 14.00 15394 544
721 27.01 19189 542	
751 25.01 22637 35	557 25.01 22845 55
78 23.01 18293 447	12 25.01 23785 50
1192 13.00 15394 135	207 14.00 15394 530
	303 25.00 704 12
594 23.01 12259 510 9	578 14.00 15394 124
618 14.00 77	613 14.00 15394 503
	702 25.01 23725 211
729 25.00 204 15	781 25.00 415 53
	827 25.01 30755 540
7 25.01 31514 486	
10 14.00 15394 450	
	277 23.01 0 723
370 22.01 5957 530	
551 23.01 15253 585	528 14.00 15394 101
565 14.00 15394 511	561 25.01 30584 523
566 14.00 15394 434	538 25.01 30584 523
	744 27.01 13104 535
	834 25.00 0 249
	593 25.01 22557 134
155 14.00 15394 52	
157 14.00 15394 427	
278 24.00 5307 723	

continuum

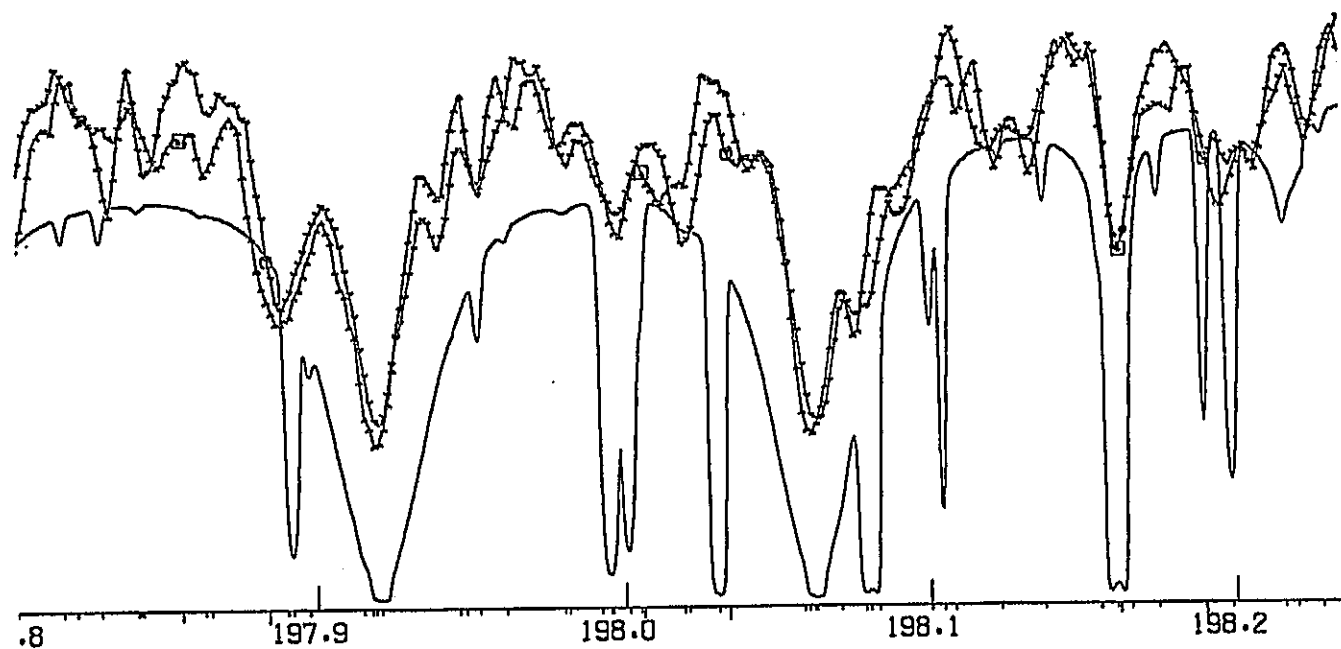


Figure 3 (Continued).

14 14.00 1534 483	227 22.01 0 723	
15 14.00 1534 483		
16 14.00 1534 483		
17 14.00 1534 483		
18 14.00 1534 483		
19 14.00 1534 483		
20 14.00 1534 483		
21 14.00 1534 483		
22 14.00 1534 483		
23 14.00 1534 483		
24 14.00 1534 483		
25 14.00 1534 483		
26 14.00 1534 483		
27 14.00 1534 483		
28 14.00 1534 483		
29 14.00 1534 483		
30 14.00 1534 483		
31 14.00 1534 483		
32 14.00 1534 483		
33 14.00 1534 483		
34 14.00 1534 483		
35 14.00 1534 483		
36 14.00 1534 483		
37 14.00 1534 483		
38 14.00 1534 483		
39 14.00 1534 483		
40 14.00 1534 483		
41 14.00 1534 483		
42 14.00 1534 483		
43 14.00 1534 483		
44 14.00 1534 483		
45 14.00 1534 483		
46 14.00 1534 483		
47 14.00 1534 483		
48 14.00 1534 483		
49 14.00 1534 483		
50 14.00 1534 483		
51 14.00 1534 483		
52 14.00 1534 483		
53 14.00 1534 483		
54 14.00 1534 483		
55 14.00 1534 483		
56 14.00 1534 483		
57 14.00 1534 483		
58 14.00 1534 483		
59 14.00 1534 483		
60 14.00 1534 483		
61 14.00 1534 483		
62 14.00 1534 483		
63 14.00 1534 483		
64 14.00 1534 483		
65 14.00 1534 483		
66 14.00 1534 483		
67 14.00 1534 483		
68 14.00 1534 483		
69 14.00 1534 483		
70 14.00 1534 483		
71 14.00 1534 483		
72 14.00 1534 483		
73 14.00 1534 483		
74 14.00 1534 483		
75 14.00 1534 483		
76 14.00 1534 483		
77 14.00 1534 483		
78 14.00 1534 483		
79 14.00 1534 483		
80 14.00 1534 483		
81 14.00 1534 483		
82 14.00 1534 483		
83 14.00 1534 483		
84 14.00 1534 483		
85 14.00 1534 483		
86 14.00 1534 483		
87 14.00 1534 483		
88 14.00 1534 483		
89 14.00 1534 483		
90 14.00 1534 483		
91 14.00 1534 483		
92 14.00 1534 483		
93 14.00 1534 483		
94 14.00 1534 483		
95 14.00 1534 483		
96 14.00 1534 483		
97 14.00 1534 483		
98 14.00 1534 483		
99 14.00 1534 483		
100 14.00 1534 483		

continuum

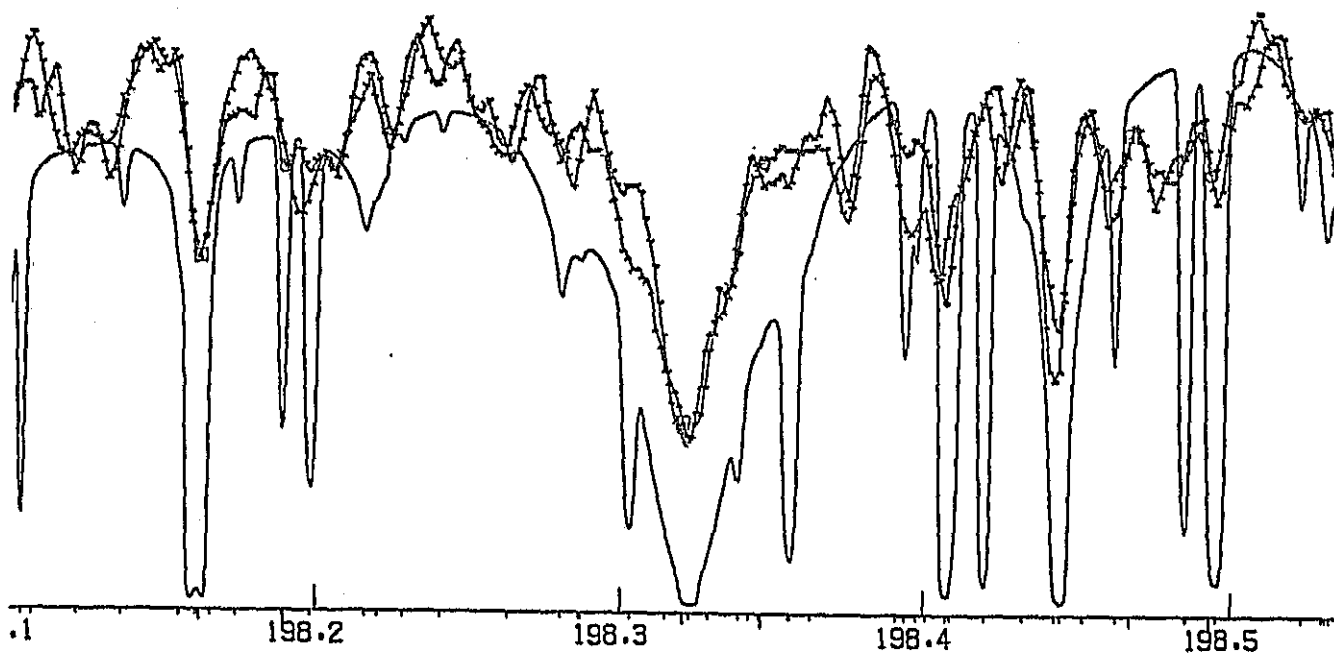


Figure 3 (Continued).

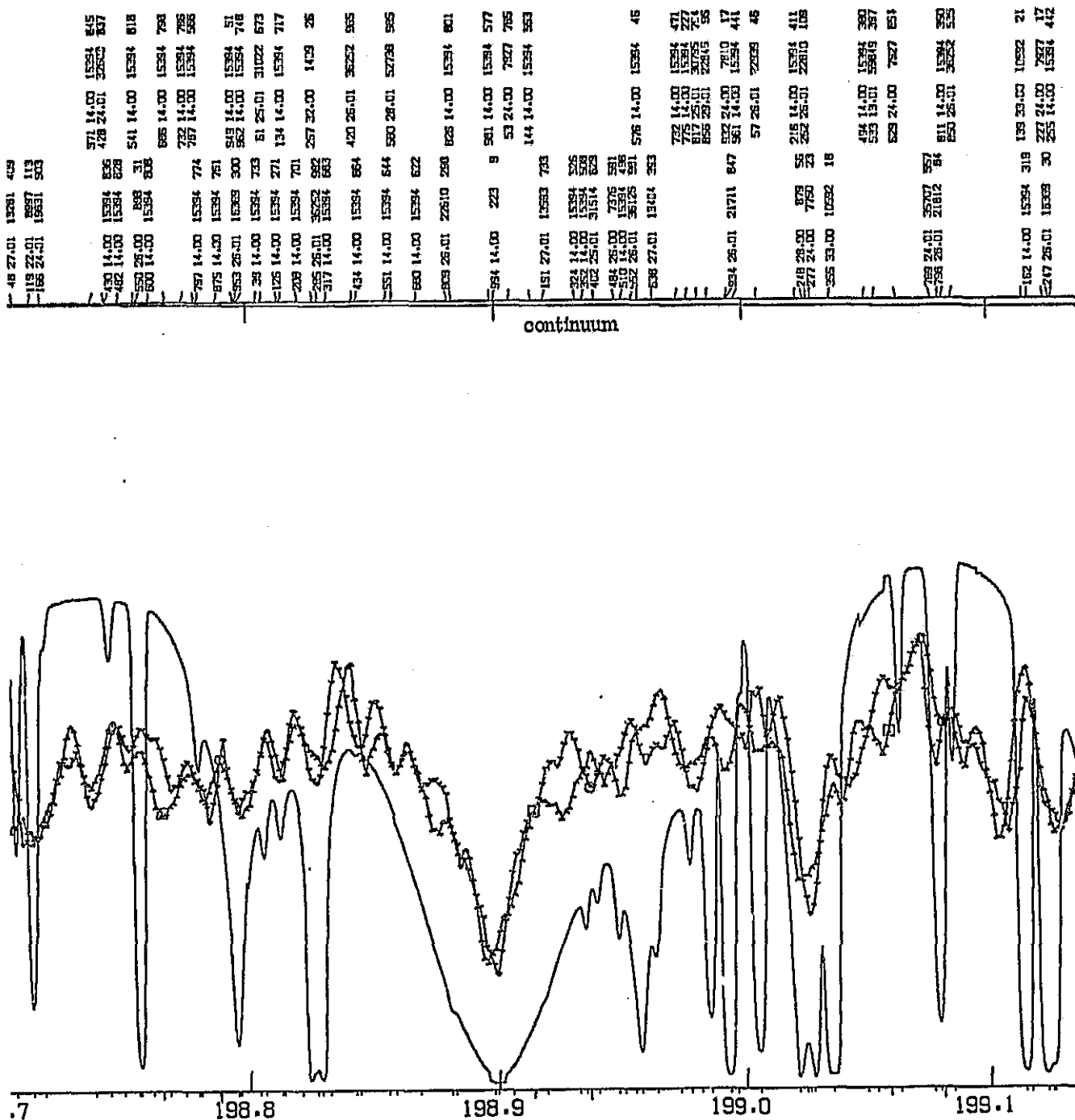


Figure 3 (Continued).

6. FURTHER WORK

We expect to make a number of improvements over the next two months, then return to NCAR for another iteration on the spectrum. Several problems that we expect to correct are the following.

C II, Mg II, Al II, and Si II lines are computed too weak because they were not based on non-LTE results. Work is underway to calculate departure coefficients for these ions.

Many highly ionized lines do not appear in the calculation. We are adding the coronal approximation to treat such lines.

There are many molecular lines in the observed spectrum. We are adding molecular lines to our line list.

For many lines like Fe II we use an approximate scattering source function in the chromosphere, but emission cores still appear in the calculation, contrary to observation. We are developing a more accurate procedure for dealing with these lines.

7. REFERENCES

- Avrett, E. H., 1971, *Journ. Quant. Spectrosc. Radiat. Transfer*, vol. 11, pp. 511-529.
- Avrett, E. H., and Loeser, R., 1969, *Smithsonian Astrophys. Obs. Spec. Rep.* No. 303, 98 pp.
- Kurucz, R. L., 1970, *Smithsonian Astrophys. Obs. Spec. Rep.* No. 309, 291 pp.
- Kurucz, R. L., 1974, *Astrophys. Journ. (Lett.)*, vol. 188, pp. L21-L22.
- Kurucz, R. L., and Peytremann, E., 1975, *Smithsonian Astrophys. Obs. Spec. Rep.* No. 362 (in 3 parts), 1219 pp.
- Vernazza, J. E., Avrett, E. H., and Loeser, R. 1973, *Astrophys. Journ.*, vol. 184, pp. 605-631.
- Vernazza, J. E., Avrett, E. H., and Loeser, R., 1976, *Astrophys. Journ. Suppl. Series*, vol. 30, pp. 1-60.